Simulations of thin semi-flexible polymers

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We present an alternative approach [1] suitable for simulations of semi-flexible polymers. In contrast with the usual bead-rod compromise between bead-spring and rigid rod models, we use deformable cylindrical segments as basic units of the polymer. The length of each segment is not preserved with end points diffusing under constraints keeping the polymer chain nature intact. The model allows the simulation of tension propagation and elasticity properties. In particular, we describe a new cooperative regime in the relaxation of the polymer from its fully elongated configuration.

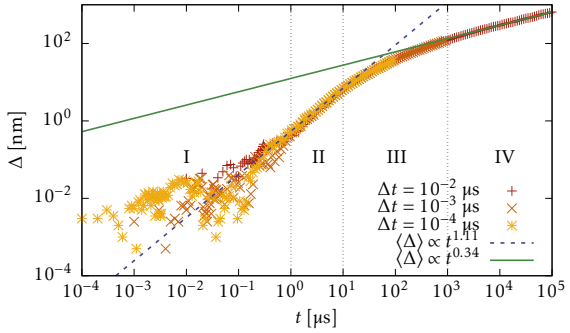

Figure 1: Log-log plot of the time dependency of the polymer's end point displacement Δ during the relaxation from $T = 0$ K. The newly described cooperative regime is denoted by II.

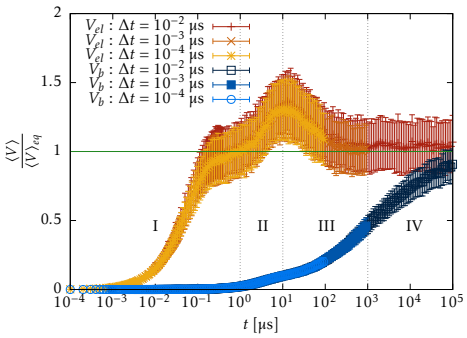

Figure 2: Semi-log plot of the mean bending $\langle V_b \rangle$ and elastic $\langle V_{el} \rangle$ energy during the relaxation from $T = 0$ K demonstrating the cooperative nature of the new regime II.

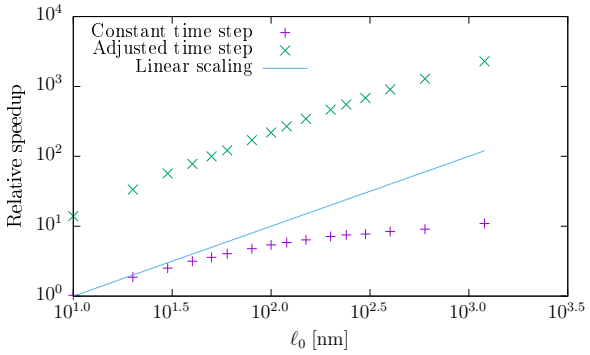

Figure 3: The dependency of the speed-up of our model relative to the bead-spring model with respect to the equilibrium segment length ℓ_0.

References

[1] Jiří Pešek, Pieter Baerts, Bart Smeets, Christian Maes and Herman Ramon *Mathematical model suitable for efficient simulations of thin semi-flexible polymers in complex environments*, Soft Matter **12**, 3360–3387, 2016. DOI: 10.1039/C5SM03106K

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